Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Comparison between α- and β-carbonic anhydrases : could $Zn(His)_3(H_2O)$ and $Zn(His)(Cys)_2(H_2O)$ enzymes sites be equivalents ?

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A) Computational methods..... S2

B) Comparison between optimized and crystal structures of α- and β-CA..... S6

C) Structural parameters for **α-X⁻** and **β-X⁻** (X=1-5)..... ..... S7

D) Absolute energies for all models..... ..... S8

E) Cartesian coordinates..... ..... S8

A) Computational methods

1- DFT level

We use a well established methodology,[1] the GGA density functional BP86,[2] to optimize all of our geometries. These geometry optimizations were accelerated using the Resolution of Identity (RI) approximation method,[3] as implemented in Turbomole.[4] The geometry optimizations for models **5** were further accelerated using the Multipole Accelerated Resolution of Identity for J (MARI-J) approximation method.[5] Basis sets of split-valence quality, def2-SVP (and abbreviated SVP),[6] and the associated auxiliary basis sets to fit Coulomb potentials,[7] were employed for all atoms in the geometry optimization. In order to hold the structures sufficiently close to the X-ray structure, α-carbons have been fixed at their position in the X-ray analysis (see below).

Improved energies were obtained by single-point calculations at the B3LYP level,[8] with the extended basis set of valence triple zeta quality, labeled def2-TZVPP (and abbreviated TZVPP).[7,9] For models **5**, full B3LYP/TZVPP calculations were not possible due to computational limitations as the number of Atomic Orbitals exceed 10000. Thus, a mixed TZVPP (for all atoms included in models **4**) and SVP basis set (for all others atoms) has been used, leading to 7022 and 6531 AOs for **α-5H** and **β-5H** respectively. For an additional gain in speed, the resolution of identity (RI) approximation was used.

We have used these levels of calculations in our former studies.[10] They have been shown to give reliable geometries and relative energetic data for zinc complexes as compared with other density functionals or post-HF calculations.[1d,11]

Solvation free energy corrections were determined using the conductor-like screening model (COSMO)[12] which is a polarizable continuum solvation model. The COSMO calculations were carried out on the gas-phase BP86/SVP geometries, at the B3LYP/TZVPP level, with dielectric constants ε of 78.4.

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Binding energies of the zinc-bound water molecule and of the zinc dication have been computed at the gas-phase BP86/SVP geometries of the whole system, without re-optimisation of the fragments. They have been corrected to basis set superposition error (BSSE) by the well established counterpoise method.
Accurate absolute pKa values could not be obtained from our calculations. However, high level DFT calculations with polarized continuum model solvent corrections have been shown to provide a balanced treatment for the calculation of relative pK_a values for metal-bound water ligands.[13] This has be achieved through the use of the following equation which gives the expected relative pK_a values from relative PA values :

$$\Delta \mathrm{p}K_\mathrm{a} = \frac{\Delta \mathrm{PA_{solv}}\ (\mathrm{kJ/mol})}{5.71}$$

The constant 5.71 = $RT\log_e(10)$, in kJ/mol

2- Computed models

Our computational models **1-5** have been built from X-ray structures of representatives members of the α-CA and β-CA classes (PDB 2CBA and 1G5C respectively). For 1G5C, we select the zinc site of chain B as it includes a zinc-bound water molecule and no hepes group. For models **1-4**, we have selected molecular groups step-by-step, based on their location and chemical influence. These groups included amino-acid side chain, backbone amide group, amino-acid, peptide or water molecules located in the neighbouring of zinc. For models 5, we have included all chemical groups located at a distance lower than 9 Å of the zinc atom. In all cases, model **n** includes model **n-1**. When an amino-acid side chain is selected, all the side chain from the C_α atom is included in the model, thus allowing fixing this atom in its position in the X-ray structure. When an amino-acid or a peptide is selected, the side-chains have been either conserved, simplificated (for example Thr to Ser) or replaced by an H atom, depending on their position and chemical influence. Furthermore, C- and N-termination of amino-acids and peptides have been capped by -N(H)-$C_\alpha H_3$ and -C(O)-$C_\alpha H_3$ groups. Thus, in all cases, backbone amide group, amino-acids and peptides have C_α atoms at their two extremities, which are fixed.

Models **1** include the zinc dication, the coordinated water molecule (W263 and W2 for α and β respectively) and the first coordination shell of the metal (side chains of His94, His96 and His119 for α, side chains of Cys32, His87 and Cys90 for β). Models **α-1H** and **β-1H** include thus 49 and 35 atoms respectively.

Models **2** include models **1** and the second coordination shell around protein Zn-ligands. For **α-2**, this corresponds (i) to the side chain of Gln92, hydrogen bonded to His94; (ii) to the backbone amide group between Asn244 and Trp245, hydrogen bonded to His96; (iii) to the side chain of Glu117 and the peptide Glu106-His107, forming a hydrogen bond network around His119. For **β-2**, this corresponds (i) to the backbone amide group betwen Ala58 and Gly59, and the simplificated peptide Cys32-Met33Gly, both hydrogen bonded to Cys32; (ii) to the simplificated peptide His87-Thr88Gly-Asp89Gly-Cys90-Gly91 and the water molecule W33, forming a hydrogen bond network around His87 and Cys90. Models **α-2H** and **β-2H** include thus 118 and 101 atoms respectively.

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It should be noted that, through the -N(H)-$C_\alpha H_3$ capped group of Gly91, the NH amide group of Met92 is included in **β-2** as it is hydrogen bonded to the S-thiolate of Cys90. Model **β-2** thus also includes the amide group located between Cys90 and Gly91 to "close" the protein backbone and to be chemically pertinent. However, this second NH amide group is hydrogen bonded to the zinc-bound water molecule, and thus should only be part of model **β-3** and larger. In order to evaluate the influence of this interaction, we also built a modified model, noted **β-2'**, in which this amide group located between Cys90 and Gly91 has been replaced by two hydrogen atoms. The obtained structural parameters and energetic properties are presented in Table S1.

Table S1. structural parameters and energetic properties of model **β-2'**
Mains structural parameters for compounds **β-2'H**

	Zn-O	*Zn-L_1*	*Zn-L_2*	*Zn-L_3*	*Σ(X-O-X)*
β-2'H	2.188	2.283	2.058	2.293	326.3

Energetic properties for compounds **β-2'**

	PA_{gaz}[b]	*PA_{solv}*[b]	*$BE(H_2O_{(Zn)})$*[c]	*BE(Zn)*[c]
β-2'	1315	1240	50	2807

These data show that this hydrogen bond induces a noticeable increase of the Zn-O bond length (2.188 and 2.274 Å in **β-2'H** and **β-2H** respectively) but does not modify significantly any of the energetic data.

Models **3** include models **2**, the "gatekeeper" and its surrounding. For **α-3**, the "gatekeeper" corresponds to the Thr199Ser amino-acid and the side chain of Glu106. Its surroundings include the amide group between Trp245 and Arg246 and W265. For **β-3**, the "gatekeeper" corresponds to the side chain of Asp34 and the peptide Ser35Gly-Arg36. Its surroundings include W17 and the side chain of Asp89. It should be noted that we decided to protonate the side chain of Asp89 to take into account the electronic surroundings of the carboxylate group as it is hydrogen bonded to the side chain of Arg16 (from chain A) and close to the side chain of Arg94. This protonated Asp89 is conserved in **β-4** but not in **β-5** which includes both arginines. Models **α-3H** and **β-3H** include thus 152 and 146 atoms respectively.

Models **4** include models **3** and the remaining chemical groups directly located around the zinc-bound water molecule. For **α-4**, this includes W318 and W338 (called "deep water"), both hydrogen bonded to $H_2O_{(Zn)}$, the amide group between Leu198 and Thr199, and the side chain of Thr200Ser. For **β-4**, this includes W167, hydrogen bonded to $H_2O_{(Zn)}$, W117 and W22. Models **α-4H** and **β-4H** include thus 169 and 155 atoms respectively.

Models **5** include models **4** and all the remaining chemical groups located in a sphere with a radius of 9 Å and centered on zinc.
Models **α-5**, depicted in figure S1, is built with the zinc Zn262, the side chain of Tyr7 and Trp209, the peptides Ser29-Pro30, Ala65-Phe66Gly-Asn67, Gln92-Phe93Gly-His94-Phe95-His96, Ser105-Glu106-His107, Glu117-Leu118-His119-Leu120Gly-Val121, Val143-Leu144Gly-Gly145, Ser197-Leu198Gly-Thr199-Thr200-Pro201 and Asn244-Trp245Gly, and the water molecules W263, W264, W265, W292, W295, W318, W319, W338, W359, W369, W381, W389, W393 and W461. Besides α-carbons, all atoms except H from the side chain of

Tyr7 and Trp209 have been fixed in their position in the X-ray structure, which lead to 60 frozen atoms (58 C, 1 O and 1 N) during the optimisation process. Model **α-5H** includes thus 530 atoms.

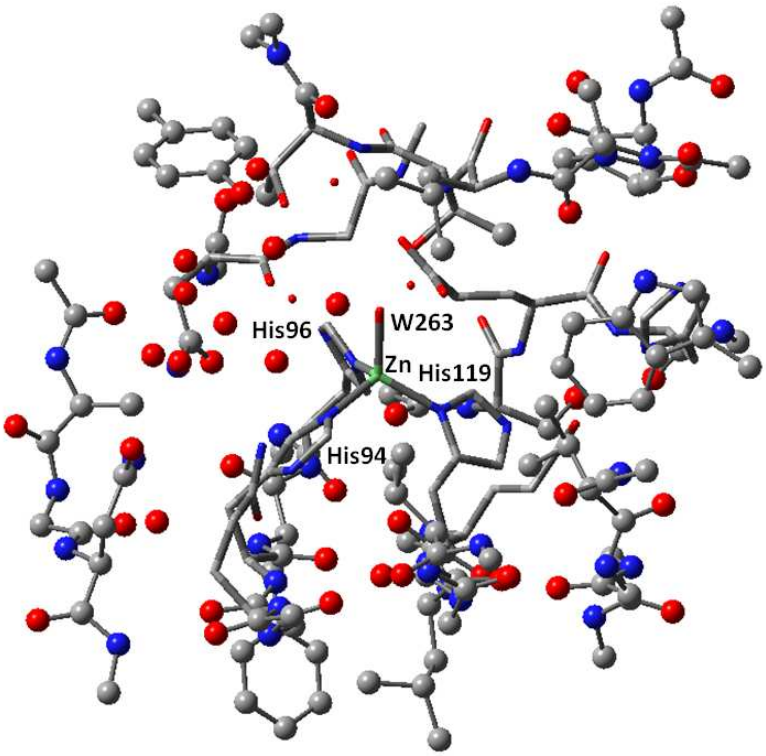


Figure S1. Optimized structure of **α-5H** at the BP86/SVP level. The **α-4H** part is depicted in "Tube" whereas the remaining atoms are depicted in "Ball & Stick". The H atoms have been omitted for clarity.

Models **β-5**, depicted in figure S2, is built with the zinc Zn1002 of chain B, the side chain of Ser19 (chain A), Lys53 (chain A), Leu77 (chain A), Asn131 (chain B), Ile158 (chain B), the amino-acid Glu128 (chain B), the peptides Arg16-Asp17 (chain A), Thr31-Cys32-Met33-Asp34-Ser35-Arg36-Leu37 (chain B), Asn57-Ala58-Gly59-Asn60-Ile61 (chain B), Val85Gly-Gly86-His87-Thr88Gly-Asp89-Cys90-Gly91-Met92-Ala93-Arg94 (chain B), and the water molecules W2, W17, W19, W22, W33, W35, W114, W117, W167, W181, W194, W234 and W295. Besides α-carbons, all atoms except H from the side chain of Leu77 and Ile158 have been fixed in their position in the X-ray structure, which lead to 45 frozen atoms (all C) during the optimisation process. Model **β-5H** includes thus 494 atoms.

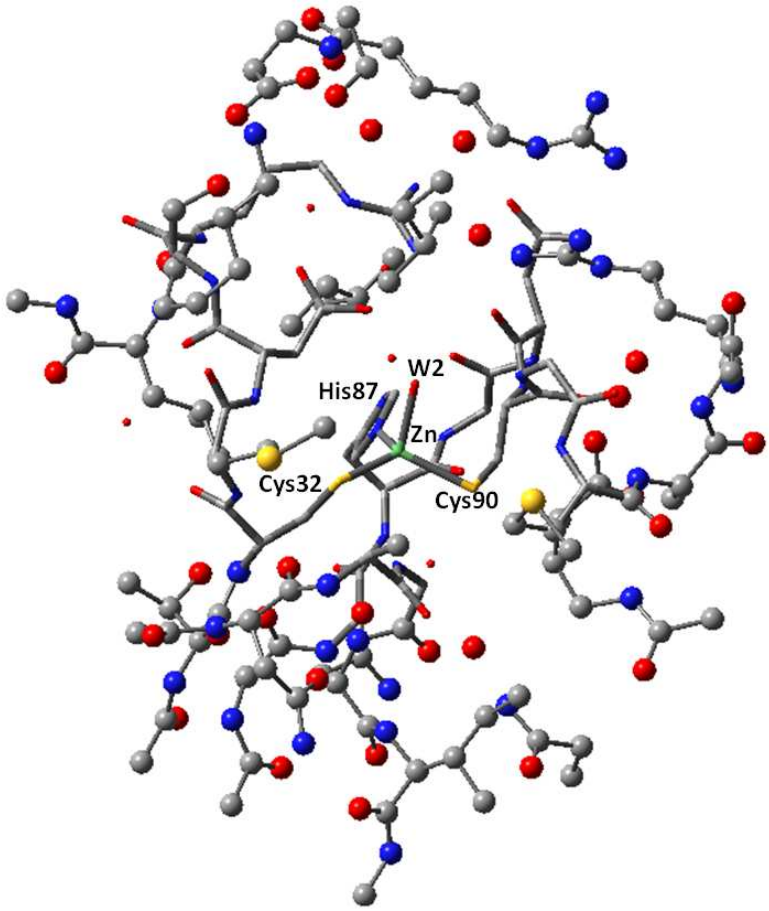


Figure S2. Optimized structure of **β-5H** at the BP86/SVP level. The **β-4H** part is depicted in "Tube" whereas the remaining atoms are depicted in "Ball & Stick". The H atoms have been omitted for clarity.

B) Comparison between optimized and crystal structures of α- and β-CA.

The comparison between BP86/SVP optimized structures of all our models and corresponding part of crystal structures (PDB 2CBA and 1G5C) of α- and β-CA enzymes is presented in Table S2.

Table S2. Structural parameters for deprotonated compounds **1-5** as determined by geometry optimisation at the BP86/def2-SVP level of calculation.

	Full model[a]	*Zn core*[b]
α-1H	0.354	0.354
α-2H	0.468	0.215
α-3H	0.545	0.205
α-4H	0.420	0.149
α-5H	0.395	0.123
β-5H	0.459	0.125
β-4H	0.353	0.190
β-3H	0.251	0.182
β-2H	0.231	0.229
β-1H	0.639	0.639

[a] RMSD values computed for all atoms, except H, in models **α/β-XH**.
RMSD values computed only for atoms included in models **α/β-1H**.

RMSD values have been used to estimate the quality of our optimized structures compare to experiment. As shown in Table S3, the optimized structures are close to the

experimental one. There are some minor discrepancies between the experimental and the optimized for the whole systems, due mainly to the residues and water molecules located at the outside part of each model. On the opposite, the zinc active site of the protein is well reproduced, and the larger the used models (from **1** to **5**), the better the quality of our optimized structures to reproduce the zinc core.

C) Structural parameters for α-X$^-$ and β-X$^-$ (X=1-5)

Table S3. Structural parameters for deprotonated compounds **1**-**5** as determined by geometry optimisation at the BP86/def2-SVP level of calculation.

	Zn-O[a]	*Zn-L*$_1$[a,b]	*Zn-L*$_2$[a,c]	*Zn-L*$_3$[a,d]
α-1$^-$	1.887	2.051	2.060	2.059
α-2$^-$	1.872	2.075	2.073	2.070
α-3$^-$	1.858	2.115	2.043	2.103
α-4$^-$	1.910	2.069	2.036	2.083
α-5$^-$	1.933	2.023	2.027	2.035
β-5$^-$	1.993	2.394	2.117	2.361
β-4$^-$	1.933	2.364	2.160	2.368
β-3$^-$	1.918	2.375	2.151	2.382
β-2'$^-$	1.931	2.373	2.137	2.368
β-2$^-$	1.920	2.377	2.130	2.394
β-1$^-$	1.960	2.355	2.228	2.349

[a] bond lengths (Å). [b] L_1 = N(His94) / S(Cys32) for α- / β-CA respectively. [c] L_2 = N(His96) / N(His87) for α- / β-CA respectively. [d] L_3 = N(His119) / S(Cys90) for α- / β-CA respectively. [e] Sum of the Zn-O-H and H-O-H angles (°).

D) Absolute energies for all models

Table S4. Absolute electronic energies and solvation free energies corrections for all models in u.a.

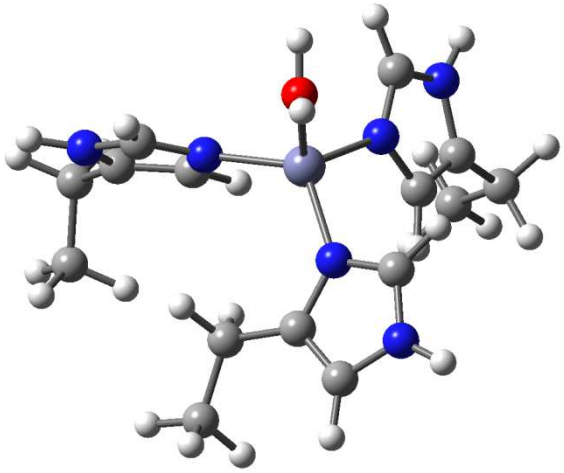
Structure	E[a]	E[b]	$G^{78.4}_{corr}$[c]	E(system-H_2O)[d]	E(H_2O)[e]	E(system-Zn)[f]	E(Zn)[g]
α-1H	-2769.387080	-2769.731578	-0.226972	-2693.260735	-76.431118	-990.730392	-1778.320502
α-1⁻	-2769.078391	-2769.425377	-0.073610				
β-1H	-3115.105891	-3115.344175	-0.031955	-3038.899728	-76.429999	-1335.839914	-1778.320089
β-1⁻	-3114.538810	-3114.787653	-0.106823				
α-2H	-4333.054027	-4334.157484	-0.120879	-4257.695165	-76.431236	-2554.927206	-1778.320536
α-2⁻	-4332.640262	-4333.751908	-0.079465				
β-2'H	-4895.024853	-4896.185526	-0.096816	-4819.735368	-76.431222	-3116.796143	-1778.320317
β-2'⁻	-4894.523835	-4895.684670	-0.125544				
β-2H	-5062.418676	-5063.665230	-0.105675	-4987.215471	-76.431404	-3284.291656	-1778.320315
β-2⁻	-5061.934776	-5063.180757	-0.130286				
α-3H	-5246.796173	-5248.380837	-0.095701	-5171.880861	-76.411636	-3468.957255	-1778.320554
α-3⁻	-5246.266926	-5247.872373	-0.140147				
β-3H	-6332.027584	-6333.923778	-0.134192	-6257.447220	-76.423157	-4554.533381	-1778.320487
β-3⁻	-6331.520973	-6333.417167	-0.167121				
α-4H	-5721.916048	-5723.781086	-0.109217	-5647.268050	-76.417556	-3944.367056	-1778.320615
α-4⁻	-5721.415414	-5723.291508	-0.141292				
β-4H	-6561.197070	-6563.252218	-0.134714	-6486.766764	-76.424781	-4783.847649	-1778.320546
β-4⁻	-6560.675411	-6562.743026	-0.181203				
α-5H	-14909.226064	-14905.276937	-0.174177	-14828.764150	-76.417374	-13125.885433	-1778.320719
α-5⁻	-14908.716770	-14904.773883	-0.196738				
β-5H	-14802.027109	-14799.087751	-0.200345	-14722.611871	-76.427603	-13019.694342	-1778.320547
β-5⁻	-14801.524383	-14798.578144	-0.231158				

[a] absolute energy of models **1-5** at the ri-BP86/def2-SVP level (marij-BP86 for models 5).
[b] absolute energy of models **1-5** at the ri-B3LYP//def2-TZVPP//ri-BP86/def2-SVP level (mixed TZVPP and SVP basis set for models 5).
[c] correction to solvation free energy in water (ε= 78.4) at the COSMO-ri-B3LYP//def2-TZVPP//ri-BP86/def2-SVP level (mixed TZVPP and SVP basis set for models 5).
[d] Counterpoise absolute energy of models **1H-5H** without the zinc-bound water molecule at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).
[e] Counterpoise absolute energy of the zinc-bound water molecule at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).
[f] Counterpoise absolute energy of models **1H-5H** without the zinc dication at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).
[g] Counterpoise absolute energy of the zinc dication at the ri-B3LYP//def2-TZVPP level (mixed TZVPP and SVP basis set for models 5).

E) Cartesian coordinates

Model α-1H

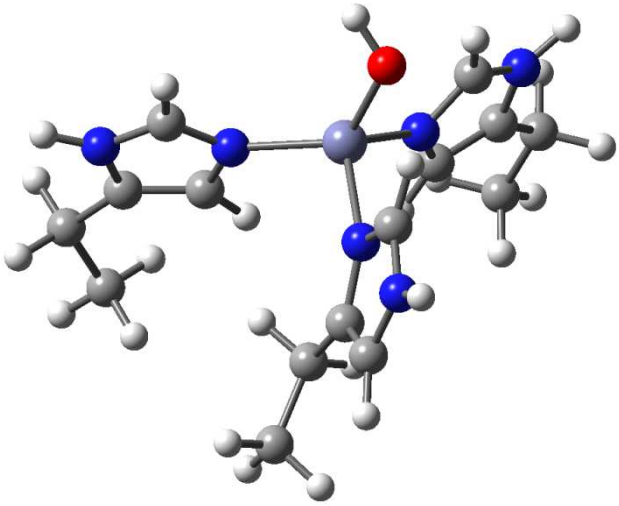
O	-15.1945871	14.9479409	22.0873037
Zn	-14.6689737	13.1145095	22.9480787
N	-16.1502394	11.7570087	22.8960621
C	-17.4475549	11.8578576	23.2189575
N	-17.9906665	10.6192589	23.2989539
C	-17.0228089	9.6624358	23.0212422
C	-15.8759600	10.3986674	22.7681175
C	-17.2576965	8.1850518	23.1156059
C	-17.0132740	7.6225650	24.5317940
N	-14.3411416	13.5712461	24.8681959
C	-14.4503446	12.6274533	25.8821423
C	-14.0207062	13.1761794	27.0805955
N	-13.6561435	14.4752900	26.7519616
C	-13.8567915	14.6884318	25.4284150
C	-13.8596672	12.5751684	28.4459363



C	-12.6593800	11.6110050	28.5452740
N	-13.1644041	12.5711147	21.7362644
C	-13.2710362	12.3928255	20.4070007
N	-12.0929984	11.9564721	19.9136265
C	-11.1881153	11.8402950	20.9525591
C	-11.8575239	12.2263553	22.1017410
C	-11.3633745	12.2963031	23.5180278
C	-9.9693200	11.7002250	23.7325670
H	-12.7669873	10.7579257	27.8463253
H	-9.9347197	10.6287412	23.4511584
H	-15.9662265	7.7873399	24.8544965
H	-11.7034622	12.1240640	28.3192675
H	-17.2047601	6.5320720	24.5465919
H	-9.6762010	11.7745745	24.7968113
H	-18.0101967	12.7814116	23.3946674
H	-18.9731747	10.4209934	23.5131974
H	-18.2921551	7.9548231	22.7841138
H	-16.5883049	7.6824539	22.3887396
H	-17.6829616	8.0893057	25.2819958
H	-12.5860458	11.1991965	29.5704732
H	-13.7631327	13.3889335	29.1943807
H	-14.7952641	12.0377463	28.7052614
H	-14.8290402	11.6163063	25.6982675
H	-13.3060441	15.1744275	27.4145684
H	-13.6546107	15.6379277	24.9207375
H	-11.3706684	13.3612041	23.8432516
H	-12.0986604	11.7793427	24.1739064
H	-9.1987898	12.2372335	23.1437291
H	-10.1607756	11.4990090	20.7955904
H	-11.9044816	11.7406855	18.9298300
H	-14.1676730	12.5527546	19.7972001
H	-14.8808223	10.0271921	22.5011936
H	-14.6671291	15.4022597	21.4011321
H	-16.0139219	15.4697728	22.1948813

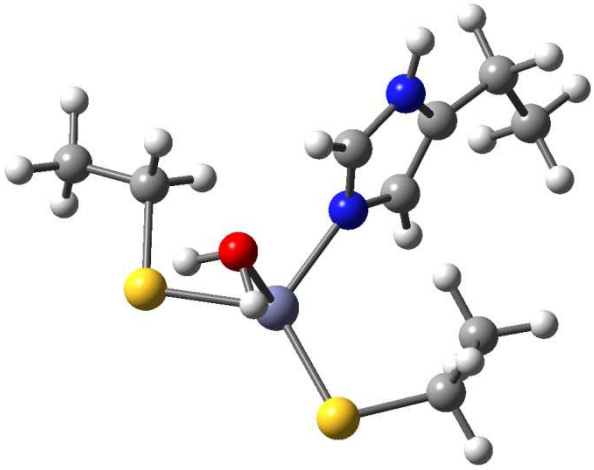
Model α-1^{-}

O	-15.8449653	14.5526726	22.0674366
Zn	-14.8839780	13.4415327	23.2513721
N	-16.0347618	11.7337312	23.2184923
C	-17.1143075	11.8989218	22.4501171
N	-17.8672810	10.7689694	22.4718772
C	-17.2550628	9.8241137	23.2894902
C	-16.1061112	10.4534050	23.7438167
C	-17.8272533	8.4590412	23.5380217
C	-17.0132740	7.6225650	24.5317940
N	-14.3832273	13.8768808	25.1918195
C	-14.0032845	12.9588798	26.1575564
C	-13.5357301	13.6198884	27.2820777
N	-13.6556076	14.9671437	26.9645610
C	-14.1629602	15.0859284	25.7076346
C	-12.9871828	13.1093756	28.5815109
C	-12.6593800	11.6110050	28.5452740
N	-13.1088521	13.3204195	22.2157221
C	-13.1227960	14.0330331	21.0846775
N	-11.9079003	13.9622936	20.4885692
C	-11.0769662	13.1747028	21.2710913
C	-11.8392470	12.7720928	22.3571352
C	-11.4735935	11.8991015	23.5243617
C	-9.9693200	11.7002250	23.7325670
H	-13.5644391	11.0010122	28.3507453
H	-9.4973717	11.1984640	22.8633268
H	-15.9799788	7.4508495	24.1681100
H	-11.9100818	11.3792583	27.7623709
H	-17.4826683	6.6310959	24.6791826
H	-9.7752977	11.0645375	24.6184431
H	-17.3088024	12.8341786	21.9002757
H	-18.7452005	10.6363908	21.9655181
H	-18.8722161	8.5667063	23.9063590
H	-17.9076417	7.9166340	22.5690838
H	-16.9528168	8.1158741	25.5229980
H	-12.2458916	11.2824848	29.5179492
H	-12.0740791	13.6897013	28.8406456
H	-13.7146949	13.3176027	29.3978909
H	-14.0886134	11.8807414	25.9946994
H	-13.4002377	15.7469400	27.5748360
H	-14.3466760	16.0439469	25.2080938
H	-11.9268736	12.3431889	24.4362207
H	-11.9696479	10.9096132	23.3990986
H	-9.4489767	12.6672609	23.8875306
H	-10.0377020	12.9730051	20.9970510
H	-11.6492911	14.4196899	19.6123438
H	-14.0089330	14.5926740	20.7462234
H	-15.3366204	10.0497224	24.4089077
H	-16.3215938	15.3047688	22.4598402



Model β-1H

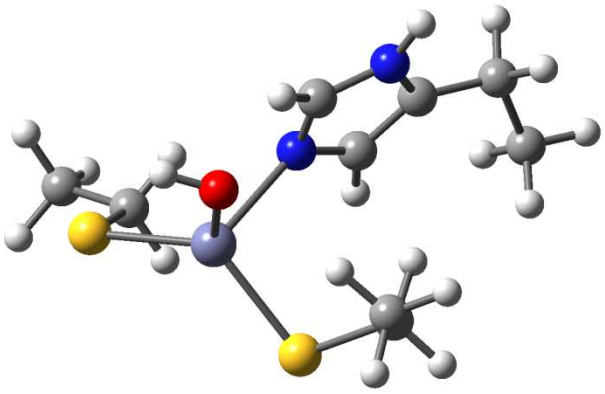
C	-16.2419399	45.6328016	25.9798260
C	-16.2357075	44.8416825	27.1181618
N	-17.4409283	45.1277813	27.7483889
C	-18.1221918	46.0452870	27.0073950
N	-17.4114024	46.3663446	25.9285984
C	-15.2324598	43.8623401	27.6475910
C	-14.0881150	43.6052950	26.6631430
Zn	-18.1559139	47.6907461	24.5240806
O	-20.2231508	47.8879632	25.7397500
S	-17.8046916	49.8753283	25.0819882
C	-16.9708526	49.6849726	26.7325760
C	-16.3535300	51.0060380	27.1857050



H	-17.1236030	51.8009825	27.2635114
S	-18.9998901	46.7968867	22.6335405
C	-18.5505121	45.0041131	22.7930590
C	-19.4293610	44.1986560	23.7492410
H	-13.5250344	44.5353657	26.4461217
H	-15.8682005	50.9000310	28.1801709
H	-15.5884961	51.3549836	26.4624874
H	-16.1857549	48.9045777	26.6570316
H	-17.7103602	49.3304731	27.4825205
H	-13.3697749	42.8725060	27.0794168
H	-14.8201785	44.2333792	28.6135283
H	-15.7457304	42.9042743	27.8893282
H	-17.7708350	44.7095644	28.6198249
H	-19.1146958	46.4524320	27.2380901
H	-15.4784857	45.7139030	25.1995201
H	-19.3655069	44.5969762	24.7821645
H	-18.6308607	44.5913369	21.7652931
H	-17.4814150	44.9140910	23.0780966
H	-19.8772502	48.8198243	25.6459876
H	-20.6180130	47.6959769	24.8590890
H	-20.4942430	44.2461357	23.4423163
H	-19.1243907	43.1289599	23.7715713
H	-14.4651832	43.2022008	25.7021472

Model **β-1**$^{-}$

C	-16.2843493	45.6833098	26.8626262
C	-16.2566771	44.4850415	27.5614689
N	-17.5552502	44.3350490	28.0457033
C	-18.3043642	45.4015727	27.6206250
N	-17.5458976	46.2278230	26.9115304
C	-15.1690246	43.4693704	27.7429312
C	-14.0881150	43.6052950	26.6631430
Zn	-18.8060307	47.4053419	25.5010038
O	-20.3962777	46.4981260	26.1998400
S	-18.5778321	49.6748021	26.0869479
C	-16.7948473	49.6686795	26.5748068
C	-16.3535300	51.0060380	27.1857050
H	-16.9581292	51.2416820	28.0877733
S	-17.8402535	46.5651982	23.5308881
C	-17.9951269	44.7406992	23.7814257
C	-19.4293610	44.1986560	23.7492410
H	-13.5968007	44.5979348	26.7115530
H	-15.2783669	50.9931019	27.4788469
H	-16.5064401	51.8379495	26.4653055
H	-16.1660002	49.4366683	25.6862339
H	-16.6143484	48.8509331	27.3065393
H	-13.2977259	42.8362542	26.7859992
H	-14.7011894	43.5519484	28.7532503
H	-15.6076815	42.4460044	27.7019156



H	-17.9091417	43.5265863	28.5570386
H	-19.4083848	45.5516897	27.6283962
H	-15.4912326	46.1584955	26.2748643
H	-20.0419244	44.7079109	24.5254149
H	-17.3862774	44.2554367	22.9838161
H	-17.5156333	44.4547734	24.7460217
H	-20.9656597	47.2028268	26.5629541
H	-19.9032486	44.4060954	22.7656844
H	-19.4575663	43.0961969	23.9236773
H	-14.5252865	43.5014129	25.6503258

Model **α-2H**

N	-13.0092172	10.3901736	15.8442035
C	-12.9379817	9.7474757	14.6191235
C	-13.0339554	10.7745038	13.6815866
N	-13.1550409	12.0010590	14.2977121
C	-13.1358803	11.7332222	15.5956913
C	-12.8037480	8.2598191	14.4925083
C	-14.1190300	7.4536750	14.6112320
N	-14.8064978	7.6308097	15.8650059
C	-16.1551423	7.8500191	15.9379662
O	-16.8866478	8.0576572	14.9722944
C	-16.7110760	7.8300350	17.3736580
N	-16.1231814	6.7842762	18.1916871
C	-16.8482759	5.8425913	18.8725578
C	-16.0143640	4.6255130	19.2644660
O	-18.0548710	5.9416249	19.1134337
O	-15.0712728	14.8462838	21.9509723
Zn	-14.6822823	13.0964521	23.0793640
N	-16.1915496	11.7743725	23.0421304
C	-17.5310352	11.8069161	23.1490989
N	-18.0319396	10.5517629	23.1442161
C	-16.9840287	9.6539955	23.0333667
C	-15.8403785	10.4323708	22.9688653
C	-17.1539441	8.1665880	23.0979915
C	-17.0132740	7.6225650	24.5317940
N	-14.2582016	13.7174749	24.9275900
C	-14.2116103	12.8447803	26.0063461
C	-13.6062481	13.4772367	27.0832095
N	-13.2952915	14.7487517	26.6269063
C	-13.6920798	14.8625615	25.3400123
C	-13.2930253	13.0119107	28.4784080
C	-12.6593800	11.6110050	28.5452740
N	-13.2705112	12.3604715	21.9136945
C	-13.5551537	11.7100429	20.7474815
N	-12.5109447	11.0174601	20.2826851
C	-11.4908597	11.2200477	21.1861773
C	-11.9442860	12.0465243	22.2059461
C	-11.2226793	12.5250477	23.4316058
C	-9.9693200	11.7002250	23.7325670
O	-12.7289843	9.2102424	18.5431809
C	-12.8138974	7.9568356	18.9358203
C	-12.4299372	7.6219539	20.3768083
C	-12.9703108	6.2605376	20.8272407
C	-12.5945320	5.8774640	22.2573820
O	-13.1783482	7.0613676	18.1611721
O	-12.0158036	16.3334542	28.4137061
C	-11.6245902	17.4028373	28.9187447
C	-11.2346465	17.4817857	30.3882474
C	-10.0507263	16.5592666	30.7469890
C	-8.7104820	17.0011290	30.1496800
N	-11.5200031	18.5475409	28.1976676
O	-20.5679180	9.7548467	23.3419744
C	-21.5034723	8.9602892	23.1115141
C	-22.4808780	8.5979410	24.2242620

N	-21.7107680	8.3918900	21.8956846
C	-20.9018020	8.6345760	20.7021270
H	-21.5557888	8.8647878	19.8382556
H	-13.3310928	10.8353719	28.1250484
H	-10.2148053	10.6278927	23.8693548
H	-16.0133501	7.8517272	24.9520313
H	-11.7032940	11.5723537	27.9864384
H	-12.9722370	6.6150966	22.9978492
H	-8.7332401	17.0113403	29.0395541
H	-13.8805444	6.3761204	14.4478041
H	-17.1439396	6.5222028	24.5475637
H	-8.4290563	18.0198685	30.4893447
H	-13.0136373	4.8887037	22.5316696
H	-9.4706733	12.0557737	24.6558182
H	-21.9183883	8.1187579	25.0496760
H	-23.2979294	7.9236277	23.9047470
H	-18.1501622	12.7071718	23.2293874
H	-19.0578604	10.2726826	23.1897818
H	-18.1416979	7.8903442	22.6770479
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H	-14.2288431	13.0249960	29.0796975
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H	-12.8055590	15.4820425	27.2085519
H	-13.5577987	15.7616819	24.7290192
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H	-9.9746832	16.5188136	31.8535515
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H	-12.1328615	17.1680286	30.9610699
H	-11.0116738	18.5293236	30.6816442
H	-11.1869425	19.4164451	28.6145208
H	-11.7581210	18.5477138	27.2043239
H	-10.9468058	13.5990266	23.3192356
H	-11.9137723	12.4841253	24.3019378
H	-9.2264077	11.7740395	22.9129930
H	-10.5068851	10.7585850	21.0513770
H	-12.5714346	10.0024193	19.3246756
H	-14.5398288	11.7276912	20.2619026
H	-11.4938064	5.8167229	22.3901457
H	-14.0751453	6.2675148	20.7158215
H	-12.6085899	5.4901261	20.1166144
H	-12.7706081	8.4412884	21.0462343
H	-11.3171000	7.6423473	20.4331056
H	-12.9512064	9.9296369	16.7659119
H	-13.1997963	12.4728288	16.4056437
H	-13.0155007	10.6775815	12.5878724
H	-12.0795077	7.8834880	15.2488531
H	-12.3584385	8.0261795	13.5033327
H	-14.8273945	7.7549003	13.8134537
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H	-17.8013475	7.6547782	17.3194360
H	-15.1154865	6.6146878	18.1051067
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H	-20.2511022	9.5048289	20.9003398
H	-20.2654927	7.7623085	20.4410664
H	-14.5139066	14.8434986	21.1453857
H	-15.9524138	15.1550770	21.6622558
H	-16.3641830	3.7641301	18.6587929
H	-14.9296919	4.7538234	19.0936436
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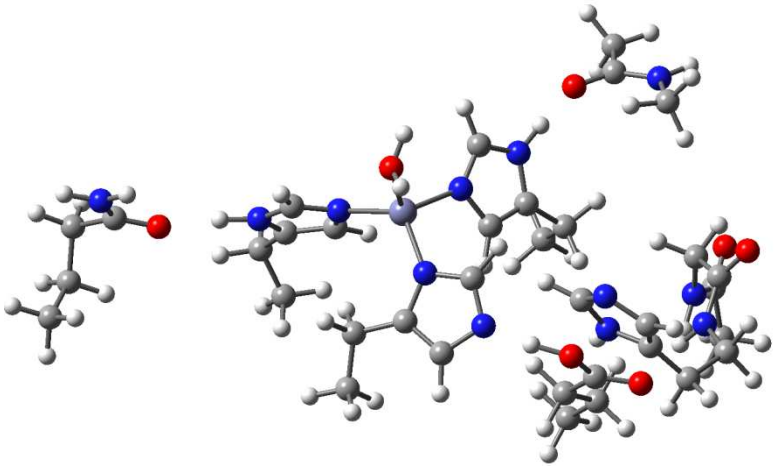

Model α-2⁻

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C	-12.8921749	10.7423885	13.7896878
N	-12.9725774	11.9586364	14.4314075
C	-12.9736157	11.6567995	15.7247331
C	-12.7682332	8.2046350	14.5427531
C	-14.1190300	7.4536750	14.6112320
N	-14.8060327	7.5920416	15.8686054
C	-16.1460853	7.8431180	15.9397578
O	-16.8711234	8.0808952	14.9721996
C	-16.7110760	7.8300350	17.3736580
N	-16.1400169	6.7962280	18.2141722
C	-16.8755999	5.7822839	18.7626007
C	-16.0143640	4.6255130	19.2644660
O	-18.1096283	5.7736262	18.8300346
O	-15.1933181	15.1447630	22.6165029
Zn	-14.7112754	13.3633288	22.9308385
N	-16.0735982	11.8011603	22.9404752
C	-17.4082250	11.8213338	23.0202759
N	-17.9011948	10.5568791	23.0734138
C	-16.8373765	9.6690710	23.0223702
C	-15.7062840	10.4672372	22.9442035
C	-16.9909069	8.1782154	23.0951817
C	-17.0132740	7.6225650	24.5317940
N	-14.1647717	13.5575655	24.9229812
C	-13.8421716	12.7373550	25.9864973
C	-13.3052263	13.5027108	27.0117793
N	-13.3193440	14.8070052	26.5377160
C	-13.8414234	14.8020182	25.2827598
C	-12.7839138	13.1259575	28.3654831
C	-12.6593800	11.6110050	28.5452740
N	-13.2307223	12.3926789	21.8583046
C	-13.5249105	11.7515361	20.7115527
N	-12.4730337	11.0383645	20.2623252
C	-11.4463397	11.2189609	21.1615073
C	-11.9111620	12.0678721	22.1572753
C	-11.1822568	12.5634006	23.3719863
C	-9.9693200	11.7002250	23.7325670
O	-12.6178317	9.1425818	18.5139755
C	-12.7979254	7.9290381	18.8960937
C	-12.3765992	7.5610355	20.3298788
C	-13.0023144	6.2585079	20.8352893
C	-12.5945320	5.8774640	22.2573820
O	-13.2775352	7.0199559	18.1695897
O	-12.0145054	16.5561067	28.3279702
C	-11.5401450	17.6524510	28.6604020
C	-11.1191933	17.9317876	30.1030425
C	-10.1459225	16.8835267	30.6758880

C	-8.7104820	17.0011290	30.1496800
N	-11.3896171	18.6780219	27.7783124
O	-20.4898547	9.6448386	23.3716475
C	-21.4746459	8.9284545	23.1215361
C	-22.4808780	8.5979410	24.2242620
N	-21.7283401	8.4122062	21.8864579
C	-20.9018020	8.6345760	20.7021270
H	-21.5299069	8.9565132	19.8479351
H	-13.6425610	11.1075993	28.4461967
H	-10.2627466	10.6451184	23.9076403
H	-16.0782551	7.8724377	25.0727075
H	-11.9766556	11.1686640	27.7917526
H	-12.8770000	6.6614838	22.9926616
H	-8.6640675	16.8790001	29.0470659
H	-13.9232364	6.3762691	14.3907941
H	-17.1197574	6.5189871	24.5248516
H	-8.2661509	17.9884601	30.3963364
H	-13.0766059	4.9319215	22.5800100
H	-9.4763365	12.0731611	24.6525831
H	-21.9446275	8.0977127	25.0542212
H	-23.3194390	7.9551902	23.8937138
H	-18.0287096	12.7245433	23.0320524
H	-18.9080113	10.2746791	23.1370820
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H	-16.1539827	7.7195604	22.5304203
H	-17.8609579	8.0427505	25.1104446
H	-12.2614944	11.3627443	29.5489740
H	-11.8006323	13.6194993	28.5237976
H	-13.4485432	13.5498600	29.1516288
H	-14.0132333	11.6566567	25.9537472
H	-12.9227599	15.6127407	27.0640538
H	-14.0122394	15.6598256	24.6149796
H	-8.0572685	16.2235573	30.5938318
H	-10.1455013	16.9795584	31.7820260
H	-10.5592758	15.8773282	30.4525092
H	-12.0615636	17.9145934	30.6919536
H	-10.6976848	18.9546553	30.2050872
H	-10.9977136	19.5764424	28.0565070
H	-11.6868834	18.5554685	26.8084412
H	-10.8633390	13.6190426	23.2151941
H	-11.8911555	12.5949017	24.2243214
H	-9.2042435	11.7059155	22.9288674
H	-10.4768831	10.7300179	21.0288412
H	-12.4914134	10.2629303	19.4740096
H	-14.4981675	11.7768525	20.2079566
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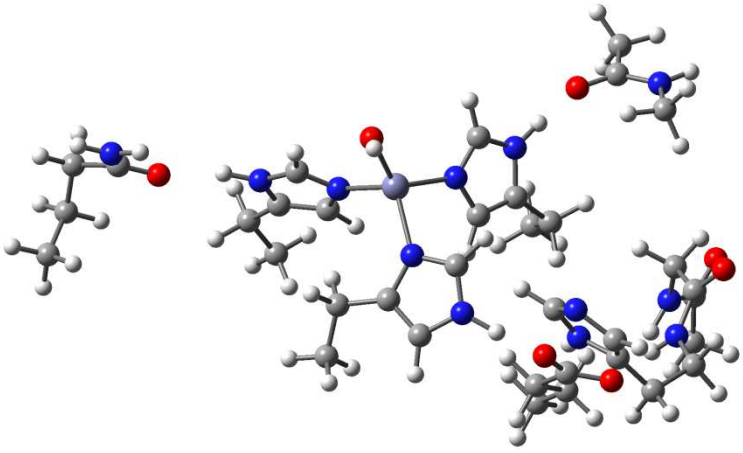
H	-14.1078902	6.3503347	20.7747896
H	-12.7376238	5.4465532	20.1277626
H	-12.6175684	8.4102981	21.0053224
H	-11.2645888	7.4882277	20.3356647
H	-12.8531480	9.8178175	16.8667190
H	-13.0200866	12.3804659	16.5501158
H	-12.8700831	10.6672864	12.6937892
H	-12.0802174	7.7772177	15.3053470
H	-12.3121031	7.9781709	13.5561041
H	-14.8073449	7.8240180	13.8242460
H	-14.2399403	7.4096398	16.7208503
H	-17.8005261	7.6528276	17.3082549
H	-15.1118478	6.7192180	18.2570300
H	-22.8863569	9.5480269	24.6242378
H	-14.6573651	10.1593456	22.8767852
H	-22.5493479	7.8135319	21.7853327
H	-20.1784999	9.4360490	20.9353000
H	-20.3396603	7.7238903	20.4045242
H	-14.7741911	15.4643533	21.7966289
H	-16.3085799	3.7148012	18.7038589
H	-14.9301331	4.7929796	19.1311038
H	-16.2352262	4.4234816	20.3321665
H	-16.5616220	8.8431191	17.8157552



Model **β-2'H**

C	-16.5474101	45.8869423	27.1096220
C	-16.2563067	44.6059710	27.5512834
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C	-18.3853767	44.7317700	26.9197077
N	-17.8712771	45.9500629	26.7131934
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C	-14.0881150	43.6052950	26.6631430
C	-14.8954573	42.6846669	25.7436512
N	-14.9733971	41.3893816	26.1717638
C	-15.8280850	40.4435160	25.4960100
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C	-20.8177650	48.9625140	29.4766230
H	-21.3281741	49.2794261	30.4074881
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C	-18.1650390	44.9424269	23.3451885
C	-19.4293610	44.1986560	23.7492410
C	-22.7275480	45.5430110	22.4402840
C	-22.5348577	46.1701172	21.0674724
N	-21.3467486	46.8367140	20.8992006
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N	-18.2674113	51.2523541	23.0838546
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H	-20.8566096	48.5821813	19.7897723
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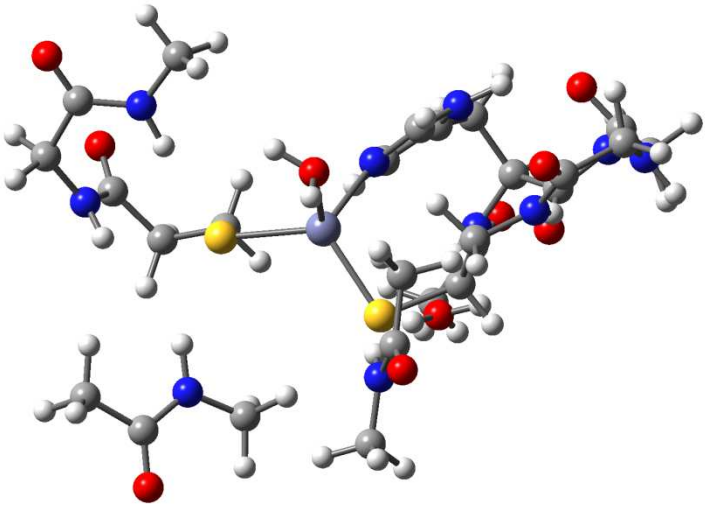

Model β-2'⁻

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C	-14.9581283	43.9461997	27.9197412
C	-14.0881150	43.6052950	26.6631430
C	-14.8606914	42.6763328	25.7226714
N	-14.9748984	41.3864654	26.1780995
C	-15.8280850	40.4435160	25.4960100
C	-17.3128493	40.6792375	25.7485531
N	-18.0835992	40.3044644	24.6941127
C	-19.5110720	40.4839330	24.6657580
H	-19.8730180	40.4629681	25.7145197
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O	-20.5773481	46.3713770	26.0976375
S	-18.5566044	49.5847739	26.0048869
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C	-16.3535300	51.0060380	27.1857050
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C	-20.3113137	51.3666804	29.4619107
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C	-20.8177650	48.9625140	29.4766230
H	-20.2579547	48.4938081	30.3175703
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C	-18.1193744	44.9244030	23.4430917
C	-19.4293610	44.1986560	23.7492410
C	-22.7275480	45.5430110	22.4402840
C	-22.5410733	46.1912595	21.0776657
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C	-21.0249620	47.4929680	19.6508800
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C	-12.2650038	45.1140537	26.0613749
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C	-11.8563090	46.3648040	25.2852440
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O	-21.1499269	41.8552210	23.5428250
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O	-15.3879205	43.0269827	24.6607478
O	-17.7511393	41.1278503	26.8144498
O	-21.0693395	51.6296296	30.4009613
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N	-18.2484859	51.2696747	23.0863940
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H	-20.6924837	53.2184273	22.7911692
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H	-15.3185003	45.0482017	23.7151977
H	-15.9817347	46.4502357	23.7877705
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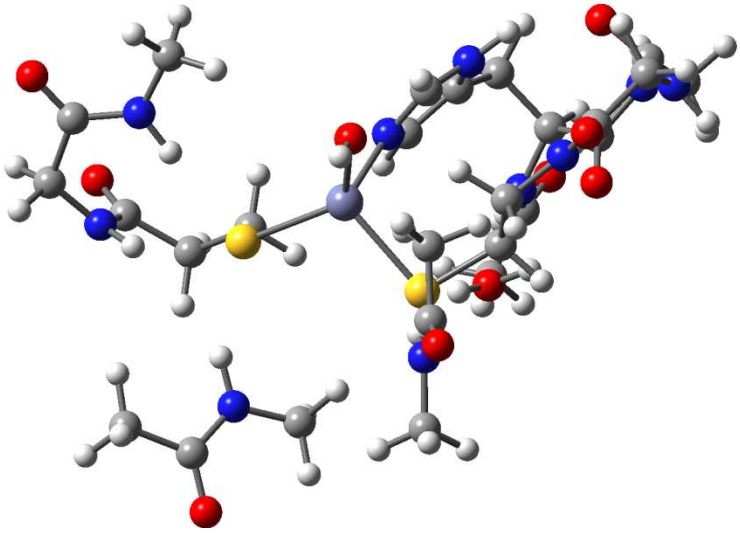

Model β-2H

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C	-14.0881150	43.6052950	26.6631430
C	-14.8505345	42.6725900	25.7179577
N	-15.0123359	41.4010647	26.2002763
C	-15.8280850	40.4435160	25.4960100
C	-17.3196567	40.6850977	25.6733260
N	-18.0828269	40.2709824	24.6312109
C	-19.5110720	40.4839330	24.6657580
H	-19.9623263	40.0252035	25.5676517
Zn	-18.5502468	47.2787228	25.3412252
O	-20.7974398	47.1325536	25.6569026
S	-18.4215256	49.4524244	26.0594776
C	-16.7272513	49.5612814	26.8202486
C	-16.3535300	51.0060380	27.1857050
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C	-19.4968300	52.4967190	28.7877220
C	-20.3485587	51.3747020	29.4277177
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C	-19.9141458	41.9773989	24.7012131
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O	-23.5521944	46.4563009	20.3807769
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O	-17.8054630	41.1957894	26.6910904
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H	-20.0879381	48.1913809	29.8032909
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H	-15.1356502	43.0526161	28.5355656
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H	-18.3421768	42.3926750	23.4304437
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H	-15.2205535	44.9220992	23.6453065
H	-15.9132254	46.3219303	23.5723721
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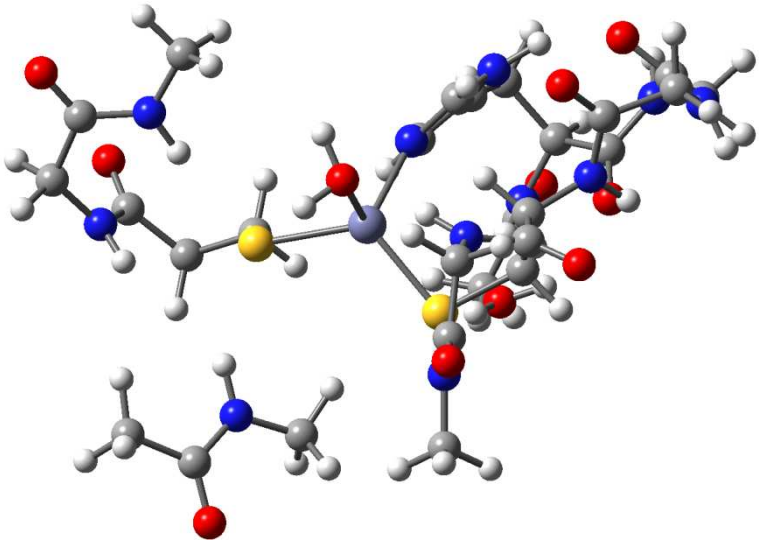

Model β-2⁻

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C	-14.0881150	43.6052950	26.6631430
C	-14.7704436	42.6441425	25.6830729
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C	-15.8280850	40.4435160	25.4960100
C	-17.3224261	40.6472690	25.7016692
N	-18.0867540	40.2313939	24.6599060
C	-19.5110720	40.4839330	24.6657580
H	-19.9902360	39.9920887	25.5347994
Zn	-18.9101295	47.2839205	25.3673138
O	-20.6940540	46.5474646	25.4381526
S	-18.5276488	49.5339420	26.0186930
C	-16.8450219	49.5871774	26.8117902
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C	-17.2000307	51.7282119	28.2549147
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C	-18.1354800	44.8613753	23.2463602
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O	-16.7680616	51.9730805	29.3820498
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C	-19.8615006	41.9908827	24.7881468
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O	-20.7738770	43.6236736	21.8138412
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O	-15.0808779	42.9290563	24.5240817
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O	-21.0507760	51.6329982	30.4168154
H	-20.0974546	48.1727414	29.7796468
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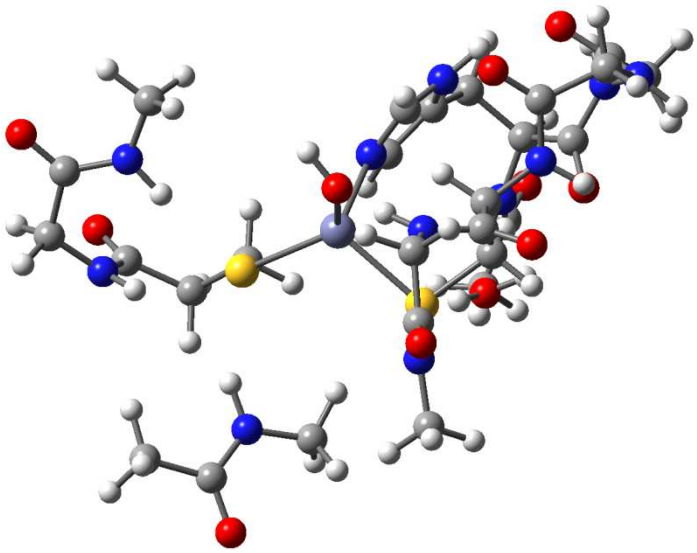

Model α-3H

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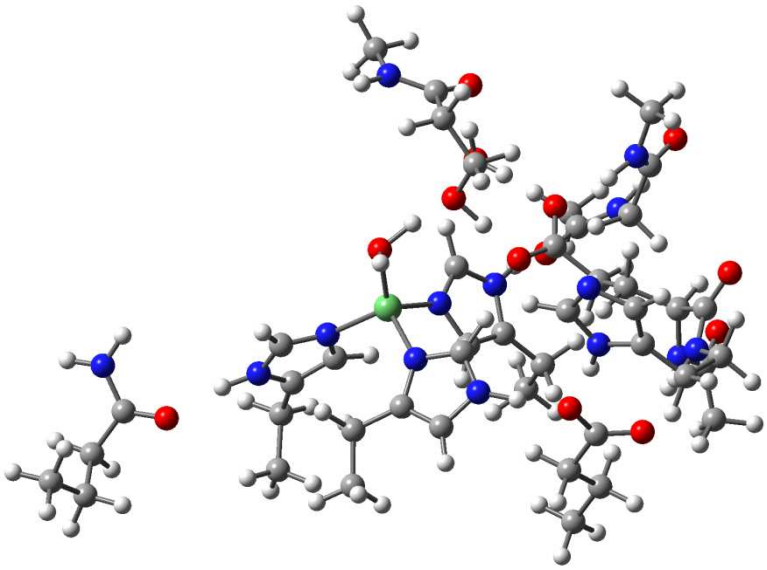

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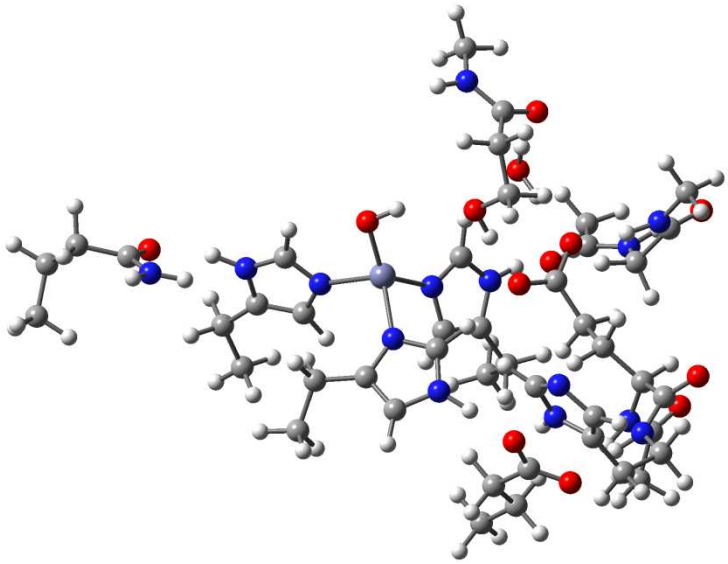

Model **β-3H**

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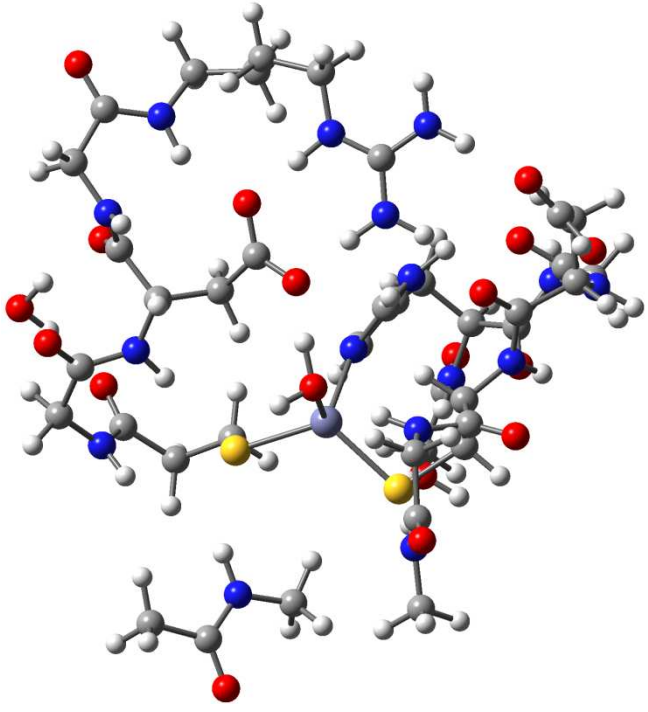

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Model β-3^{-}

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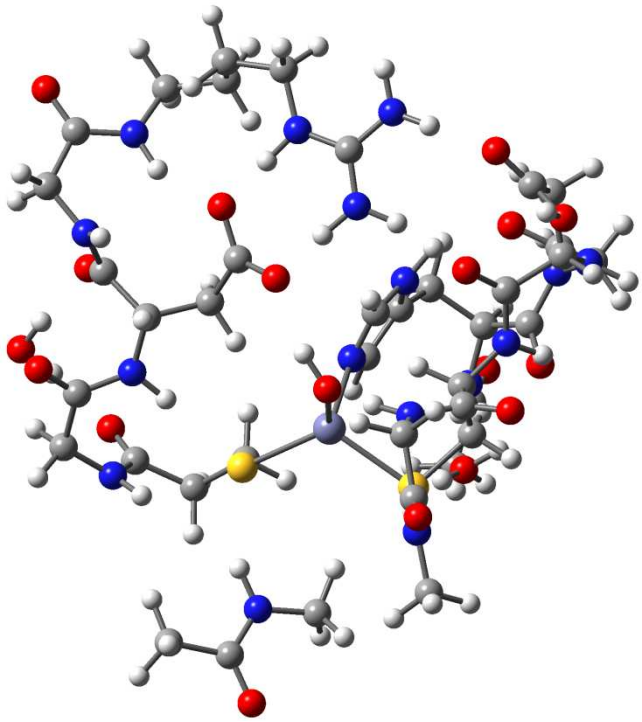

Model α-4H

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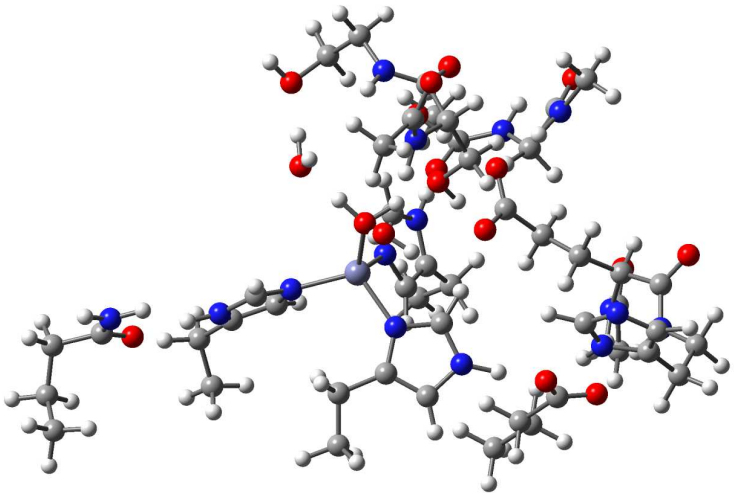

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Model α-4^{-}

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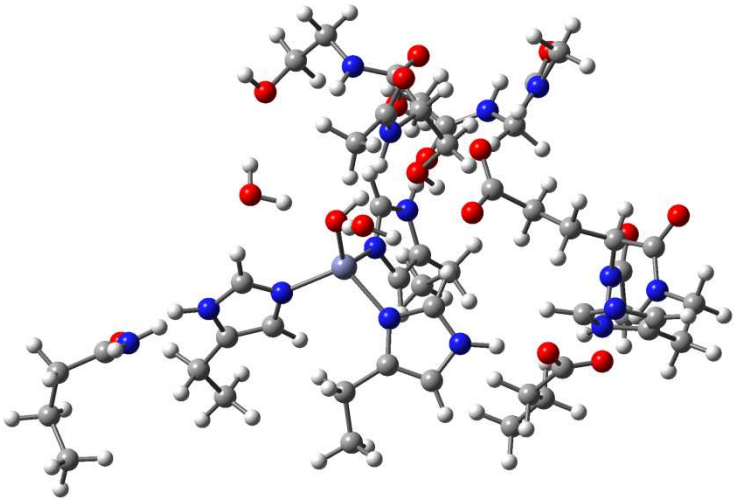

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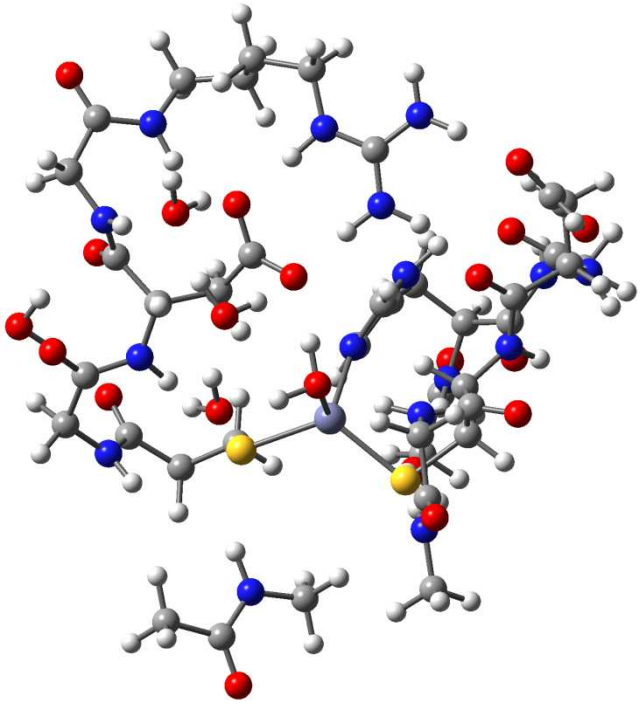

Model β-4⁻

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C	-16.3535300	51.0060380	27.1857050
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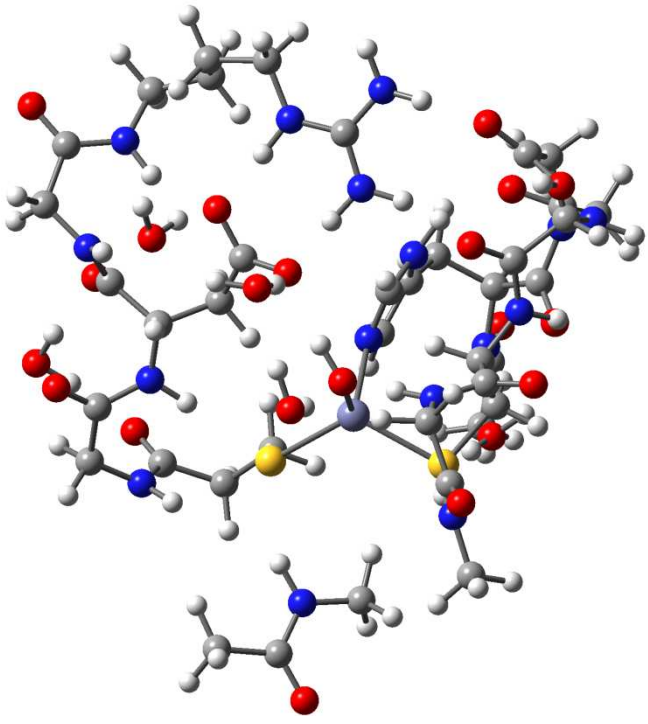

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Cartesian coordinates for models **5** could be obtained upon request to the authors.